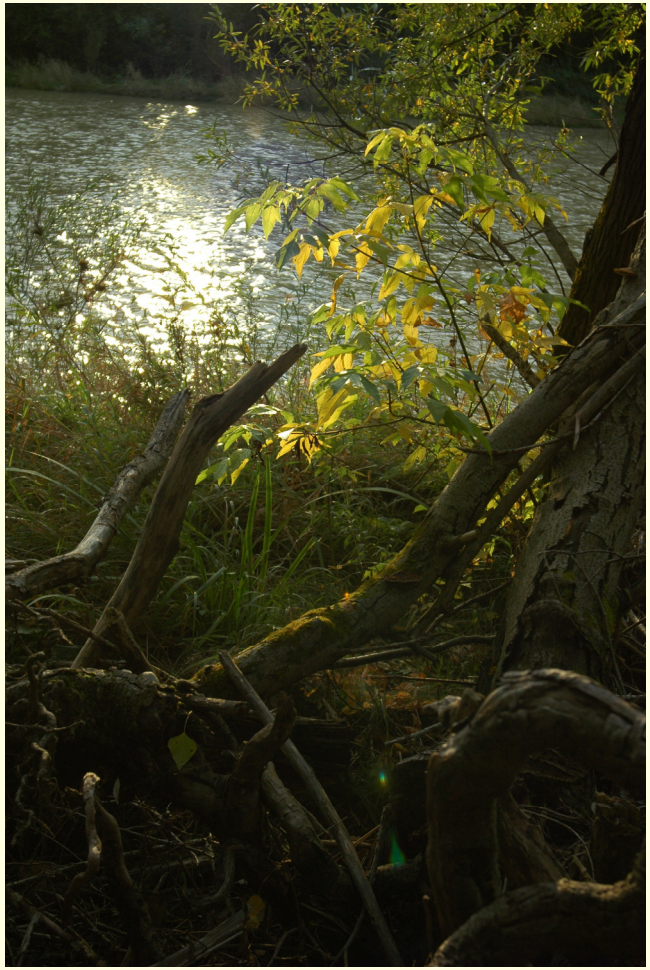
CADASTER Workshop on the use of QSAR models in REACH

Maribor, September 1-2, 2011

Panel Discussion

Friday, 2nd September
Hotel Habakuk, Maribor



Dr. Mojca Kos Durjava, PHI Maribor

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Panel Discussion

What are that major barriers for a wider use of alternative and in particular in silico methods in REACH?

Willie: The experts are not using alternatives, especially not QSARs a lot.

Etje: There are no real barriers, C&L cut off values, if the industry can have higher value with testing, they will do it.

Tomas: Uncertainty in testing is not aknowledged.

Dr. Mojca Kos Durjava, PHI Maribor

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What is your experience with use of in silico methods for REACH?

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As a regulator, which criteria will be important for you to accept the in silico model results?

Emil: Mechanistical reasoning

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As an industry, will you be willing to share your experimental data for QSAR/QSPR models development for REACH?

After REACH it is easier, now it is financial issue. It is too expensive to buy data.

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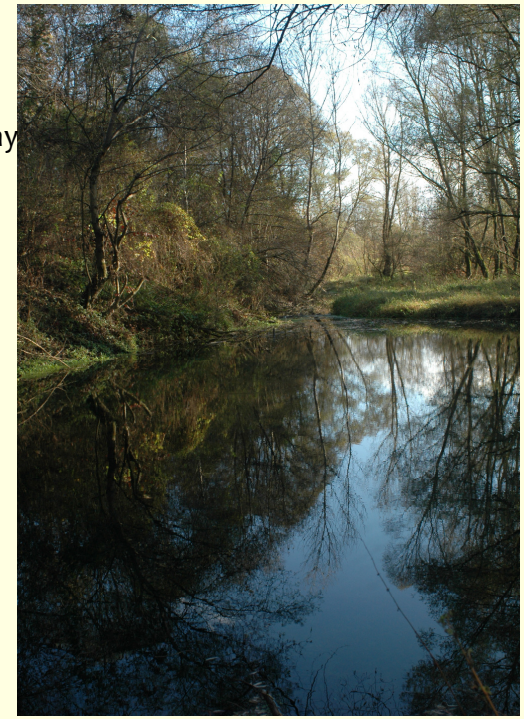
What are your recommendations and how can we improve our tools?

Barry: QSAR expert should write the new guidance, to be in touch with the science today and not 10 years ago.
The industry it takes too much time to use all of the tools, the guidance should be clear and short.



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Panel Discussion

Etje Hulzebos, IFF

When Daphnia (and algae) can also predict fish toxicity this would limit fish testing.

Which modes of actions for the 4 groups which may result in additional fish toxicity compared to algae and daphnia?

Paola: (B)TAZ good correlation between fish and algae and daphnia toxicity
Not for other classes.
Can be used tp extrapolate from daphnia to fish.

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The uncertainty of QSAR results becomes important when they are close to the cut off values of C&L and PBT assessment because of regulatory implications.

Because under REACH safe use of chemicals needs to be ensured via risk characterisation the regulatory implications on C&L may become less important but not for PBT?

Etje: C&L may be the restriction for using of QSARs

PNEC characteristaion, PBT assessment, C&L and risk characterisation: Different requirements, cut-off values

You want to be really certain in some values, that is why sometimes QSAR you are close to the cut-off value they are not useful at all.

Emil: It is not a problem to use QSARs or not, it depends on the case

Paola: PBT assessment, published

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Can the BCF models predict the BCF of reactive chemicals (e.g hydrolysing (esters) or protein binders) or readily biodegradable chemicals to potentially decrease the probability for bioaccumulation?

Willie: No

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It seems there is a lack of environmental data and most of the CADASTER QSAR models developed are an animal toxicity models.

What can be done to connect these two, any suggestion from REACH/ECHA?

Evelin: Dossiers are published on ECHA.

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Regarding proprietary data from industry:
Can't it be used to use models keeping data and model still proprietary to predict the properties?

The statistics of the model could be shown to know the model is valid.

Tomas: You must see the transparency of the model, calculation behind the model.
It is a problem, it is a political question, not scientific.

HVC data will be available.

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Andrew Worth, JRC

Is there a future for traditional QSAR in regulatory toxicology?

Andrew: Concern

Barry: Reposition is important, we need a new approach

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